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Spontaneous curvature-induced dynamical instability of Kirchhoff filaments: Application to DNA kink deformations

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Abstract

The Kirchhoff elastic theory of thin filaments with spontaneous curvature is employed in the understanding of the onset of the kink transitions observed in short DNA rings. Dynamical analysis shows that when its actual curvature is less than some threshold value determined by the spontaneous curvature, a circular DNA will begin to buckle to other shapes. The observable and the dominant deformation modes are also determined by dynamical instability analysis, and the different effects of Zn^{2+} and Mg^{2+} ions on DNA configurational properties are qualitatively discussed.

This paper is motivated mainly by a recent experiment on short DNA rings.[1,2] In this experiment, Han *et al.* synthesized a kind of DNA sequences known to have intrinsic bending tendency (in its undistorted state this kind of sequences will form an axial bend of at least 30° per helical turn.[3]) They used these sequences to investigate whether DNA can actually be kinked (forming large bendings over only few base pairs) and, if kinks really turn up, what are the necessary conditions to produce them.[1,2] Kink deformation has been theoretically proposed to be a very important mechanism for wrapping DNA around the nucleosome particles ever since the seventies,[4–6] and a recent x-ray crystalline structure of nucleosome core particle also demonstrated that DNA is not uniformly bent but has maximal and minimal curvatures at different positions.[7] However, there had been no direct evidence for the existence of kinks in DNA before the experiment of Han *et al.*[1,2] which clearly demonstrate this. To their great surprise, they found that kink formation is closely related to total chain length and solvent ionic conditions. For DNA circles with 168 base pairs (bps) or 16 helical turns, the chain is often kinked and form polygonal shapes if the solution has an appropriate Zn^{2+} or Zn^{2+}/Mg^{2+} concentrations. However, kink transition does not take place in Mg^{2+} solution alone or in Zn^{2+}/Mg^{2+} solution with high concentration of Mg^{2+} ions. For DNA circles of 126-bp or 12 helical turns, no kink will ever occur, no matter what kind of solvent ionic conditions.[1,2] Trying to interpret their novel observations, Han *et al.* suggested that axial stresses exist in 168-bp DNAs and they are the main reason for the observed kink deformations.

In this article we attempt to check, from a theoretical point of view, the validity of this insight and try to understand the radically different roles played by Mg^{2+} and Zn^{2+} ions in DNA kink transition. The spontaneous curvature[3] of the DNA material used is anticipated to play a significant role and we model the DNA chain as a thin Kirchhoff elastic filament[8] with spontaneous curvatures, i.e., adjacent cross-sections of the filament are tilted a certain angle with respect to each other (in a mean-field sense). The filament will curve to a planar ring of curvature κ_0 in its natural undistorted state, as what is observed in experiments.[3] Our study shows that a nonzero spontaneous curvature is required for the onset of the kink transitions observed in short DNA rings, in consistency with the insight of Han *et al.*

We define a moving orthonormal coordinate system $\{\mathbf{d}_1(s,t), \mathbf{d}_2(s,t), \mathbf{d}_3(s,t)\}$ along the filament axis line, with $\mathbf{d}_3$ being the tangential unit vector at arc length s. In general the filament configuration will change with time t,[9,10] so the direction vectors are also functions of t. The choice of the other two unit vectors $\mathbf{d}_1$ and $\mathbf{d}_2$ is arbitrary as long as $\mathbf{d}_1 \times \mathbf{d}_2 = \mathbf{d}_3$; in our case we define $\mathbf{d}_1$ to point to the tilt direction of the filament cross-section at each arc length point s, for convenience. Then the free energy functional of such a filament is equivalent to the following form

$$H = \frac{EI}{2} \int \left((\Omega_1 - \kappa_0)^2 + \Omega_2^2 + \Gamma(\Omega_3 - \omega_0)^2 \right) ds \tag{0.1}$$

where E is the Young's modulus of the filament and I is the momentum of inertia of the filament cross-section (assumed to be circular),[11] Γ is a dimensionless parameter ranging between 2/3 and 1.[10,11] $\mathbf{\Omega} = \sum_i \Omega_i \mathbf{d}_i$ is called the twist vector, defined by the following equation

$$\mathbf{d}_i' = \mathbf{\Omega} \times \mathbf{d}_i, \qquad (i = 1, 2, 3)$$

here and after $(\,)'$ means s-derivative. We have chosen such a continuous and homogeneous

model partly because of the experimental fact that kinking locations are not (or only very weakly) correlated with base pair types.[2]

In proposing Eq. (1) we have also take into account via the spontaneous twist rate ω_0 the fact that ordinary DNA can also have a linking number deficiency of 5%.[12] For DNA circles with 168 bps (16 turns), it may well have 0.8 turns of initial twist in the DNA circle; for those with 126 bps (12 turns), it may well have 0.6 turns of initial twist. However, this (possible) spontaneous twisting tendency cannot explain the above mentioned kink deformations of short DNA. The reason is the following: For an elastic filament formed by two chains interwinding around each other, such as DNA and actin, a well known model[13–15] concerning the effect of the fixed linking number shows that when the total twisting number variance ΔTw exceeds some threshold value $Tw_c = \sqrt{n^2-1}A/C \ \ (n \geq 2)$, a planar circle will buckle to the n-th deformation mode (this relation is also rederived in Appendix B), where A and C are respectively the bending and twisting persistence length (for DNA $A \simeq 50$ nm and $C \simeq 75$ nm.) If the kink deformations are indeed induced by this topological effect, then for the typical square ($n = 4$) polygonal kinked shape observed in the references[1,2] to appear the total twisting number of the 168-bp DNA ring are required to deviate from its equilibrium value up to $Tw_c = 3$ turns.[13–15] This value is almost four times the actual value of 0.8 turns. Thus it seems that the spontaneous twist will only play a neglectable role in the kink deformations of short DNA, and we feel it might be appropriate to focus on the macroscopic bending tendency of the filament by setting $\omega_0 = 0$ in Eq. 1. The results derived based on this approximation also confirm this to be reasonable, as can be seen later. To be complete, we have also listed out the general result of model (1) in the case of $\omega_0 \neq 0$ at the end of this paper (Appendix B), it reduces to the well known result in the references[13–15] for the limiting case of DNA with intrinsic twist but no intrinsic bend ($\kappa_0 = 0$).

Recently Goriely, Tabor[10] (and others) have suggested a powerful way to investigate on the dynamical properties of Kirchhoff thin filaments. We will use their procedure in studying the stabilities of model (1). Goriely and Tabor have worked out the stationary shape equations (SSEs) and the dynamical variational equations (DVEs)[10] for the simplest case of a filament without any spontaneous curvature. Here, for our purpose, we first give the SSEs and DVEs for a general Kirchhoff filament. (Since reference[10] has demonstrated a way to get the DVEs we will not waste space in writing down the detailed calculations, but only notice here that there are some typographical errors in this reference.) After the general SSEs and DVEs are obtained, we then turn back to the special case of Eq. (1).

The configurational free energy functional for a general Kirchhoff filament is[8–11]

$$H = \frac{EI}{2}\int((\Omega_1 - K_1^e)^2 + (\Omega_2 - K_2^e)^2 + \Gamma(\Omega_3 - K_3^e)^2)ds,$$

and the internal torque $\mathbf{M}$ is related to the deformation via the following constitutive equation

$$\mathbf{M} = EI(\Omega_1 - K_1^e)\mathbf{d}_1 + EI(\Omega_2 - K_2^e)\mathbf{d}_2 + EI\Gamma(\Omega_3 - K_3^e)\mathbf{d}_3,$$

here K_i^e $(i = 1, 2, 3)$ is the spontaneous curvature along the $\mathbf{d}_i$ direction. There are also internal forces $\mathbf{F}$ along the filament.[10,11] We can perform a standard scaling as listed in Eq. (19) of reference[10] to transform all the concerned quantities such as $\mathbf{M}$ and $\mathbf{F}$ into dimensionless forms. After this operation, we perform a basis perturbation operation suggested by Goriely and Tabor[10] to the stationary configuration $\mathbf{d}_i^{(0)}$ and get that

$$\mathbf{d}_i = \mathbf{d}_i^{(0)} + \epsilon\ \alpha \times \mathbf{d}_i^{(0)}, \tag{0.2}$$
$$\mathbf{F} = f_i^{(0)}\mathbf{d}_i^{(0)} + \epsilon\ (f_i^{(1)}\mathbf{d}_i^{(0)} + f_i^{(1)}\alpha \times \mathbf{d}_i^{(0)}), \tag{0.3}$$
$$\mathbf{M} = (\Omega_i^{(0)} - K_i^e)\mathbf{d}_i^{(0)} + \epsilon\ (\alpha_i'\mathbf{d}_i^{(0)} - \epsilon_{ijk}\alpha_i\Omega_j^{(0)}\Omega_k^{(0)}), \tag{0.4}$$

where $(\ )^{(0)}$ means value corresponding to the stationary state and $(\ )^{(1)}$ its first-order correction, ϵ is a small quantity. Insert Eqs. (2-4) into the Kirchhoff equations developed in references[9,10] and after a lengthy but straightforward calculation we can obtain the SSEs to be:

$$(\mathbf{F}^{(0)})'' = (f_1^{(0)}\mathbf{d}_1^{(0)} + f_2^{(0)}\mathbf{d}_2^{(0)} + f_3^{(0)}\mathbf{d}_3^{(0)})'' = 0, \tag{0.5}$$
$$(\Omega_1^{(0)} - K_1^e)' - (\Omega_2^{(0)} - K_2^e)\Omega_3^{(0)} + \Gamma(\Omega_3^{(0)} - K_3^e)\Omega_2^{(0)} = f_2^{(0)}, \tag{0.6}$$
$$(\Omega_2^{(0)} - K_2^e)' - \Gamma(\Omega_3^{(0)} - K_3^e)\Omega_1^{(0)} + (\Omega_1^{(0)} - K_1^e)\Omega_3^{(0)} = -f_1^{(0)}, \tag{0.7}$$
$$\Gamma(\Omega_3^{(0)} - K_3^e)' + K_1^e\Omega_2^{(0)} - K_2^e\Omega_1^{(0)} = 0. \tag{0.8}$$

Eqs. (5-8) determine the stationary configurations and their corresponding internal force $f_i^{(0)}$ and torque $(\Omega_i^{(0)} - K_i^e)$ distributions for a Kirchhoff filament with spontaneous curvatures. The stability of a stationary configuration is governed by the DVEs, which are the lengthy equations listed in Appendix A, Eqs. (24-29).

The SSEs and DVEs derived above can be applied in studying the dynamical properties of any kind of Kirchhoff filaments, however in this paper we will only study a very special case, the elastic energy Eq. (1), with $K_1^e = \kappa_0$ and $K_2^e = K_3^e = 0$. In this case, the SSEs Eqs. (5-8) demonstrate that the planar ring configuration is a stationary solution, with

$$\begin{aligned} &\Omega_1^{(0)} = \kappa = \text{const}, \quad \Omega_2^{(0)} = \Omega_3^{(0)} = 0, \\ &f_1^{(0)} = f_2^{(0)} = f_3^{(0)} = 0, \end{aligned} \tag{0.9}$$

where κ is the (actual) curvature of the ring. We now investigate on the dynamical stability of this ring shape. With Eq. (9), the DVEs Eqs. (24-29) reduce to

$$(f_1^{(1)})'' = \ddot{\alpha}_2, \tag{0.10}$$
$$(f_2^{(1)})'' - 2\kappa(f_3^{(1)})' - \kappa^2 f_2^{(1)} = -\ddot{\alpha}_1, \tag{0.11}$$
$$(f_3^{(1)})'' - \kappa^2 f_3^{(1)} + 2\kappa(f_2^{(1)})' = 0, \tag{0.12}$$
$$\alpha_1'' - f_2^{(1)} = \ddot{\alpha}_1, \tag{0.13}$$
$$\Gamma\alpha_3'' + \Gamma\kappa\alpha_2' + \kappa_0\alpha_2' - \kappa\kappa_0\alpha_3 = 2\ddot{\alpha}_3, \tag{0.14}$$
$$\alpha_2'' - \Gamma\kappa\alpha_3' + (1-\Gamma)\kappa^2\alpha_2 - \kappa_0\alpha_3' - \kappa_0\kappa\alpha_2 + f_1^{(1)} = \ddot{\alpha}_2. \tag{0.15}$$

Redefining the perturbation parameters as $\beta_1 = f_1^{(1)}, \beta_2 = \alpha_2, \beta_3 = \alpha_3, \beta_4 = f_2^{(1)}, \beta_5 = f_3^{(1)}, \beta_6 = \alpha_1$, the periodic solutions of this perturbation system Eqs. (10-15) are of the following form[10]

$$\beta_j = \mathrm{e}^{\sigma t}(x_j \mathrm{e}^{in\kappa s} + x_j^* \mathrm{e}^{-in\kappa s}) \quad (j = 1, \cdots, 6).$$

Inserting this into Eqs. (10-15), we get, in matrix form,

$$\widehat{\mathbf{L}}\cdot\mathbf{x} = \mathbf{0}, \tag{0.16}$$

where $\mathbf{x} = (x_1, x_2, x_3, x_4, x_5, x_6)^T$ and $\widehat{\mathbf{L}}$ is defined as

$$\widehat{\mathbf{L}} = \begin{pmatrix} \widehat{\mathbf{L}}_1 & \widehat{\mathbf{0}} \\ \widehat{\mathbf{0}} & \widehat{\mathbf{L}}_2 \end{pmatrix}$$

with $\widehat{\mathbf{0}}$ being the 3×3 zero-matrix and

$$\widehat{\mathbf{L}}_1 = \begin{pmatrix} -n^2\kappa^2 & -\sigma^2 & 0 \\ 0 & in(\Gamma\kappa + \kappa_0)\kappa & -\Gamma n^2\kappa^2 - \kappa_0\kappa - 2\sigma^2 \\ 1 & (-n^2 + 1 - \Gamma)\kappa^2 - \kappa_0\kappa - \sigma^2 & -in(\Gamma\kappa + \kappa_0)\kappa \end{pmatrix} \tag{0.17}$$

$$\widehat{\mathbf{L}}_2 = \begin{pmatrix} -1 & 0 & -n^2\kappa^2 - \sigma^2 \\ 2in\kappa^2 & -(n^2+1)\kappa^2 & 0 \\ -(n^2+1)\kappa^2 & -2in\kappa^2 & \sigma^2 \end{pmatrix} \tag{0.18}$$

Eq. (16) has non-zero solution $\mathbf{x}$ if and only if the determinant of the matrix $\widehat{L}$ equals to zero, i.e.,

$$\Delta_L = \Delta_{L_1} \cdot \Delta_{L_2} = 0, \tag{0.19}$$

where

$$\begin{aligned} \Delta_{L_1} = &-n^2(n^2-1)\kappa^4(\kappa_0^2 - (1-\Gamma)\kappa_0\kappa - \Gamma n^2\kappa^2) + \sigma^2((2+\Gamma)n^4\kappa^4 \\ &-2(1-\Gamma)n^2\kappa^4 + 3n^2\kappa_0\kappa^3 + \Gamma n^2\kappa^2 + \kappa_0\kappa + \sigma^2(2 + 4n^2\kappa^2)), \end{aligned} \tag{0.20}$$

$$\Delta_{L_2} = n^2(n^2-1)^2\kappa^6 + \kappa^2\sigma^2(n^2+1) + \kappa^4\sigma^2(n^2-1)^2. \tag{0.21}$$

Δ_{L_2} is related the excitation of $\{f_2^{(1)}, f_3^{(1)}, \alpha_1\}$ as can be inferred from Eq. (16) and the characteristics of the matrix $\widehat{\mathbf{L}}$, and its value is not related to κ_0, $\Delta_{L_2} > 0$ for any $n \geq 2$. Then to satisfy Eq. (19) we need only to consider Δ_{L_1} which is related to the excitation of $\{f_1^{(1)}, \alpha_2, \alpha_3\}$. (We note that $\Delta_{L_1}(n=1) = \Delta_{L_2}(n=1) = 0$ only for $\sigma = 0$, therefore the $n = 1$ modes are just soft modes[16] not important for the linear instability.)

Solution of $\Delta_{L_1}(\sigma) = 0$ with real positive σ identify the unstable modes of $\{f_1^{(1)}, \alpha_2, \alpha_3\}$ (these modes will be unstable because the amplitudes of the small fluctuations will grow exponentially with time.) From Eq. (20) it is evident that this condition is equivalent to require

$$g = \kappa_0^2 - (1-\Gamma)\kappa_0\kappa - \Gamma n^2\kappa^2 \geq 0. \tag{0.22}$$

The general behavior of g is shown in Fig. 1. It clearly demonstrates that only when the actual curvature κ of a ring is smaller than its spontaneous curvature κ_0 will it be possible for the ring to deform. This prediction is in agreement with the experiment of Han *et al.*,[1,2] and the threshold curvature for the n-th mode to buckle is

$$\kappa_c(n) = \frac{-1 + \Gamma + \sqrt{(1-\Gamma)^2 + 4\Gamma n^2}}{2\Gamma n^2}\kappa_0 \qquad (n \geq 2). \tag{0.23}$$

For $\kappa_0 = 0$, g is always negative and no buckling process will occur. Therefore we can conclude that (i) $\kappa_0 \neq 0$ and (ii) $\kappa < \kappa_0$ are the necessary conditions for the instability

of a ring (Fig. 1). Thus, our present work can qualitatively explain the novel phenomenon of DNA described in the introduction part: 126-bp DNA will not kink because no matter what ionic conditions its κ is always $\geq \kappa_c$; on the other hand, at some appropriate ionic conditions the curvature of a 168-bp DNA can become $< \kappa_c$, and kink deformation will be triggered.[1,2] When taking into account the possibility of nonzero ω_0 in Eq. (1), a threshold condition similar to Eq. (23) is derived in Appendix B.

At the initial stage of buckling, only $\{f_1^{(1)}, \alpha_2, \alpha_3\}$ will be excited, therefore the DNA configuration will deform out of the ring plane rather than deform in the same plane as the ring lies in. Thus in the present we can not tell whether the buckled shapes will actually evolve to the kinked ones observed in experiment.[1,2] To know this, nonlinear analysis beyond the buckling point is needed and it is very much involved to perform. However, we believe that the linear analysis we employed here has correctly described the behaviors of DNA at the onset of kinking.

Experiments[1–3] shows that Zn^{2+} ions can enhance the instability of DNA rings, while Mg^{2+} ions gives a negative effect. Comparing this with the theoretical analysis, it is reasonable for us to suggest that Zn^{2+} and Mg^{2+} ions will respectively increase and decrease the spontaneous curvature of the DNA chain. We are informed[2,3] that that Zn^{2+} mainly binds to DNA base pairs, and Mg^{2+} interacts with the back-bone phosphate ions. It might be possible that the intercalation of Zn^{2+} takes place mainly at the exposed side of the DNA ring hence causing an increase in its spontaneous curvature. The following analysis shows that the effect of Zn^{2+} to the spontaneous curvature is very significant.

The largest solution of $\Delta_{L_1}(\sigma) = 0$ changes with n at four fixed κ/κ_0 ratios are shown in Fig. 2. The possible deformation modes are obviously determined from these curves as they correspond to real positive values of σ. The value of n corresponding to the peaks of these curves (n_c) are just the most observable modes,[10] because these modes grow the fastest. At 1mM $ZnBr_2$ it is shown experimentally that $n_c \simeq 4$,[2] therefore we estimate from the solid line of Fig. 2 that $\kappa/\kappa_0 \simeq 0.25$. The value of κ_0 in Zn^{2+}-free solutions is till not precisely known, but it must be higher than $2\pi/126$ bp^{-1}.[2,3] On the other hand, in this condition 168-bp is not kinked, so we must have $\kappa \geq \kappa_c(2)$, or in other words, $\kappa_0 \leq 2\pi/90$ bp^{-1} if we set $\Gamma = 2/3$ in Eq. (23). Therefore, when there is no Zn^{2+} ions in the solution, $2\pi/126$ bp^{-1} $\leq \kappa_0 \leq 2\pi/90$ bp^{-1}, i.e., $0.55 \leq \kappa/\kappa_0 \leq 0.75$, (the threshold case $\kappa/\kappa_0 = 0.55$ is shown in the dot-dashed curve of Fig. 2.) Compare this estimate with the value 0.25 corresponding to 1mM $ZnBr_2$ we can conclude that the addition of 1mM Zn^{2+} ions makes the value of the spontaneous curvature of DNA increase at least one times.

This high efficiency of Zn^{2+} make us believe it to be possible that Zn^{2+} ions will induce spontaneous curvatures to DNAs even when they are originally linear and cause them to kink if they are loaded with stresses. This may be of vital biological significance. For example, it is known that transcription and replication of DNA occur with the participation of specific enzymes which contain the Zn^{2+} ion at the active site. And it is also found that transcription proceeds simultaneously with conformational changes of the DNA chain.[17] More investigations on this respect are deserved.

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Appendix A: The dynamical variation equations (DVEs)

The dynamical stability of a certain stationary configuration of the general Kirchhoff filament are determined by the dynamical variation equations listed below in Eqs. (24-29),[10,18] where $\ddot{(\,)}$ means second order t-derivative:

$$\begin{aligned}
\ddot{\alpha}_2 = &[(\alpha_2' - \alpha_3\Omega_1^{(0)} + \alpha_1\Omega_3^{(0)})' - \Omega_1^{(0)}(\alpha_3' - \alpha_1\Omega_2^{(0)} + \alpha_2\Omega_1^{(0)}) \\
&+\Omega_3^{(0)}(\alpha_1' - \alpha_2\Omega_3^{(0)} + \alpha_3\Omega_2^{(0)})]f_3^{(0)} \\
&- [(\alpha_3' - \alpha_1\Omega_2^{(0)} + \alpha_2\Omega_1^{(0)})' - \Omega_2^{(0)}(\alpha_1' - \alpha_2\Omega_3^{(0)} + \alpha_3\Omega_2^{(0)}) \\
&+\Omega_1^{(0)}(\alpha_2' - \alpha_3\Omega_1^{(0)} + \alpha_1\Omega_3^{(0)})]f_2^{(0)} \\
&+ 2(\alpha_2' - \alpha_3\Omega_1^{(0)} + \alpha_1\Omega_3^{(0)})(f_3^{(0)'} - f_1^{(0)}\Omega_2^{(0)} + f_2^{(0)}\Omega_1^{(0)}) \\
&- 2(\alpha_3' - \alpha_1\Omega_2^{(0)} + \alpha_2\Omega_1^{(0)})(f_2^{(0)'} - f_3^{(0)}\Omega_1^{(0)} + f_1^{(0)}\Omega_3^{(0)}) \\
&+ f_1^{(1)''} + 2f_3^{(1)'}\Omega_2^{(0)} - 2f_2^{(1)'}\Omega_3^{(0)} - f_1^{(1)}((\Omega_3^{(0)})^2 + (\Omega_2^{(0)})^2) \\
&+ f_2^{(1)}(-\Omega_3^{(0)'} + \Omega_2^{(0)}\Omega_1^{(0)}) + f_3^{(1)}(\Omega_2^{(0)'} + \Omega_3^{(0)}\Omega_1^{(0)}),
\end{aligned} \tag{0.24}$$

$$\begin{aligned}
-\ddot{\alpha}_1 = &[(\alpha_3' - \alpha_1\Omega_2^{(0)} + \alpha_2\Omega_1^{(0)})' - \Omega_2^{(0)}(\alpha_1' - \alpha_2\Omega_3^{(0)} + \alpha_3\Omega_2^{(0)}) \\
&+\Omega_1^{(0)}(\alpha_2' - \alpha_3\Omega_1^{(0)} + \alpha_1\Omega_3^{(0)})]f_1^{(0)} \\
&- [(\alpha_1' - \alpha_2\Omega_3^{(0)} + \alpha_3\Omega_2^{(0)})' - \Omega_3^{(0)}(\alpha_2' - \alpha_3\Omega_1^{(0)} + \alpha_1\Omega_3^{(0)}) \\
&+\Omega_2^{(0)}(\alpha_3' - \alpha_1\Omega_2^{(0)} + \alpha_2\Omega_1^{(0)})]f_3^{(0)} \\
&+ 2(\alpha_3' - \alpha_1\Omega_2^{(0)} + \alpha_2\Omega_1^{(0)})(f_1^{(0)'} - f_2^{(0)}\Omega_3^{(0)} + f_3^{(0)}\Omega_2^{(0)}) \\
&- 2(\alpha_1' - \alpha_2\Omega_3^{(0)} + \alpha_3\Omega_2^{(0)})(f_3^{(0)'} - f_1^{(0)}\Omega_2^{(0)} + f_2^{(0)}\Omega_1^{(0)}) \\
&+ f_2^{(1)''} - 2f_3^{(1)'}\Omega_1^{(0)} + 2f_1^{(1)'}\Omega_3^{(0)} - f_2^{(1)}((\Omega_1^{(0)})^2 + (\Omega_3^{(0)})^2) \\
&+ f_3^{(1)}(-\Omega_1^{(0)'} + \Omega_2^{(0)}\Omega_3^{(0)}) + f_1^{(1)}(\Omega_3^{(0)'} + \Omega_1^{(0)}\Omega_2^{(0)}),
\end{aligned} \tag{0.25}$$

$$\begin{aligned}
0 = &[(\alpha_1' - \alpha_2\Omega_3^{(0)} + \alpha_3\Omega_2^{(0)})' - \Omega_3^{(0)}(\alpha_2' - \alpha_3\Omega_1^{(0)} + \alpha_1\Omega_3^{(0)}) \\
&+\Omega_2^{(0)}(\alpha_3' - \alpha_1\Omega_2^{(0)} + \alpha_2\Omega_1^{(0)})]f_2^{(0)} \\
&- [(\alpha_2' - \alpha_3\Omega_1^{(0)} + \alpha_1\Omega_3^{(0)})' - \Omega_1^{(0)}(\alpha_3' - \alpha_1\Omega_2^{(0)} + \alpha_2\Omega_1^{(0)}) \\
&+\Omega_3^{(0)}(\alpha_1' - \alpha_2\Omega_3^{(0)} + \alpha_3\Omega_2^{(0)})]f_1^{(0)} \\
&+ 2(\alpha_1' - \alpha_2\Omega_3^{(0)} + \alpha_3\Omega_2^{(0)})(f_2^{(0)'} - f_3^{(0)}\Omega_1^{(0)} + f_1^{(0)}\Omega_3^{(0)}) \\
&- 2(\alpha_2' - \alpha_3\Omega_1^{(0)} + \alpha_1\Omega_3^{(0)})(f_1^{(0)'} - f_2^{(0)}\Omega_3^{(0)} + f_3^{(0)}\Omega_2^{(0)}) \\
&+ f_3^{(1)''} - 2f_1^{(1)'}\Omega_2^{(0)} + 2f_2^{(1)'}\Omega_1^{(0)} - f_3^{(1)}((\Omega_1^{(0)})^2 + (\Omega_2^{(0)})^2) \\
&+ f_1^{(1)}(-\Omega_2^{(0)'} + \Omega_3^{(0)}\Omega_1^{(0)}) + f_2^{(1)}(\Omega_1^{(0)'} + \Omega_2^{(0)}\Omega_3^{(0)}),
\end{aligned} \tag{0.26}$$

$$\begin{aligned}
\ddot{\alpha}_1 = &(\alpha_1' - \alpha_2\Omega_3^{(0)} + \alpha_3\Omega_2^{(0)})' + (\alpha_2' - \alpha_3\Omega_1^{(0)} + \alpha_1\Omega_3^{(0)})(\Gamma(\Omega_3^{(0)} - K_3^e) - \Omega_3^{(0)}) \\
&+ K_2^e(\alpha_3' - \alpha_1\Omega_2^{(0)} + \alpha_2\Omega_1^{(0)}) + \alpha_2(\Gamma(\Omega_3^{(0)} - K_3^e)' + K_1^e\Omega_2^{(0)} - K_2^e\Omega_1^{(0)}) \\
&- \alpha_3((\Omega_2^{(0)} - K_2^e)' - \Gamma(\Omega_3^{(0)} - K_3^e)\Omega_1^{(0)} + (\Omega_1^{(0)} - K_1^e)\Omega_3^{(0)}) - f_2^{(1)} - \alpha_3 f_1^{(0)},
\end{aligned} \tag{0.27}$$

$$\ddot{\alpha}_2 = (\alpha_2' - \alpha_3\Omega_1^{(0)} + \alpha_1\Omega_3^{(0)})' + (\alpha_3' - \alpha_1\Omega_2^{(0)} + \alpha_2\Omega_1^{(0)})((\Omega_1^{(0)} - K_1^e) - \Gamma\Omega_1^{(0)})$$
$$+ (\Omega_3^{(0)} - \Gamma(\Omega_3^{(0)} - K_3^e))(\alpha_1' - \alpha_2\Omega_3^{(0)} + \alpha_3\Omega_2^{(0)}) + \alpha_3((\Omega_1^{(0)} - K_1^e)' - (\Omega_2^{(0)} - K_2^e)\Omega_3^{(0)}$$
$$+ \Gamma(\Omega_3^{(0)} - K_3^e)\Omega_2^{(0)})) - \alpha_1(\Gamma(\Omega_3^{(0)} - K_3^e)' + K_1^e\Omega_2^{(0)} - K_2^e\Omega_1^{(0)}) + f_1^{(1)} - \alpha_3 f_2^{(0)}, \quad (0.28)$$

$$2\ddot{\alpha}_3 = \Gamma(\alpha_3' - \alpha_1\Omega_2^{(0)} + \alpha_2\Omega_1^{(0)})' - K_2^e(\alpha_1' - \alpha_2\Omega_3^{(0)} + \alpha_3\Omega_2^{(0)})$$
$$+ K_1^e(\alpha_2' - \alpha_3\Omega_1^{(0)} + \alpha_1\Omega_3^{(0)}) + \alpha_1((\Omega_2^{(0)} - K_2^e)' - \Gamma(\Omega_3^{(0)} - K_3^e)\Omega_1^{(0)} + (\Omega_1^{(0)} - K_1^e)\Omega_3^{(0)})$$
$$- \alpha_2((\Omega_1^{(0)} - K_1^e)' - (\Omega_2^{(0)} - K_2^e)\Omega_3^{(0)} + \Gamma(\Omega_3^{(0)} - K_3^e)\Omega_2^{(0)}) + \alpha_1 f_1^{(0)} + \alpha_2 f_2^{(0)}. \quad (0.29)$$

Appendix B: The linear instability result for Eq. (1) with nonzero ω_0

In the main text, we have focused our attention to the $\omega_0 = 0$ case of medel Eq. (1). For the general case of nonzero ω_0, following the same procedure as discussed in the main text we can obtain the threshold condition for the n-th mode to become instable. It reads

$$\kappa^9(n^2-1)n^4(n+1)^2 \times$$
$$(\kappa^2\kappa_0(\Gamma-1)(1-n^2)+\kappa\kappa_0^2(1-n^2)-\Gamma^2\omega_0^2(\kappa_0+\Gamma\kappa n^2)+\Gamma\kappa^3 n^2(n^2-1))=0. \qquad (0.30)$$

In the limiting case of $\omega_0 = 0$ (the filament has intrinsic bend but no intrinsic twist), Eq. (30) reduces to Eq. (23) of the main text. In the limiting case of $\kappa_0 = 0$ (then DNA has intrinsic twist but no intrinsic bend), Eq. (30) reduces to

$$-\Gamma\kappa^{10}n^6(n^2-1)^2\left(\Gamma^2\omega_0^2-\kappa^2(n^2-1)\right). \qquad (0.31)$$

Eq. (31) is just the same result obtained in previous references for a chain with intrinsic twist,[13–15] showing the correctness of this method.

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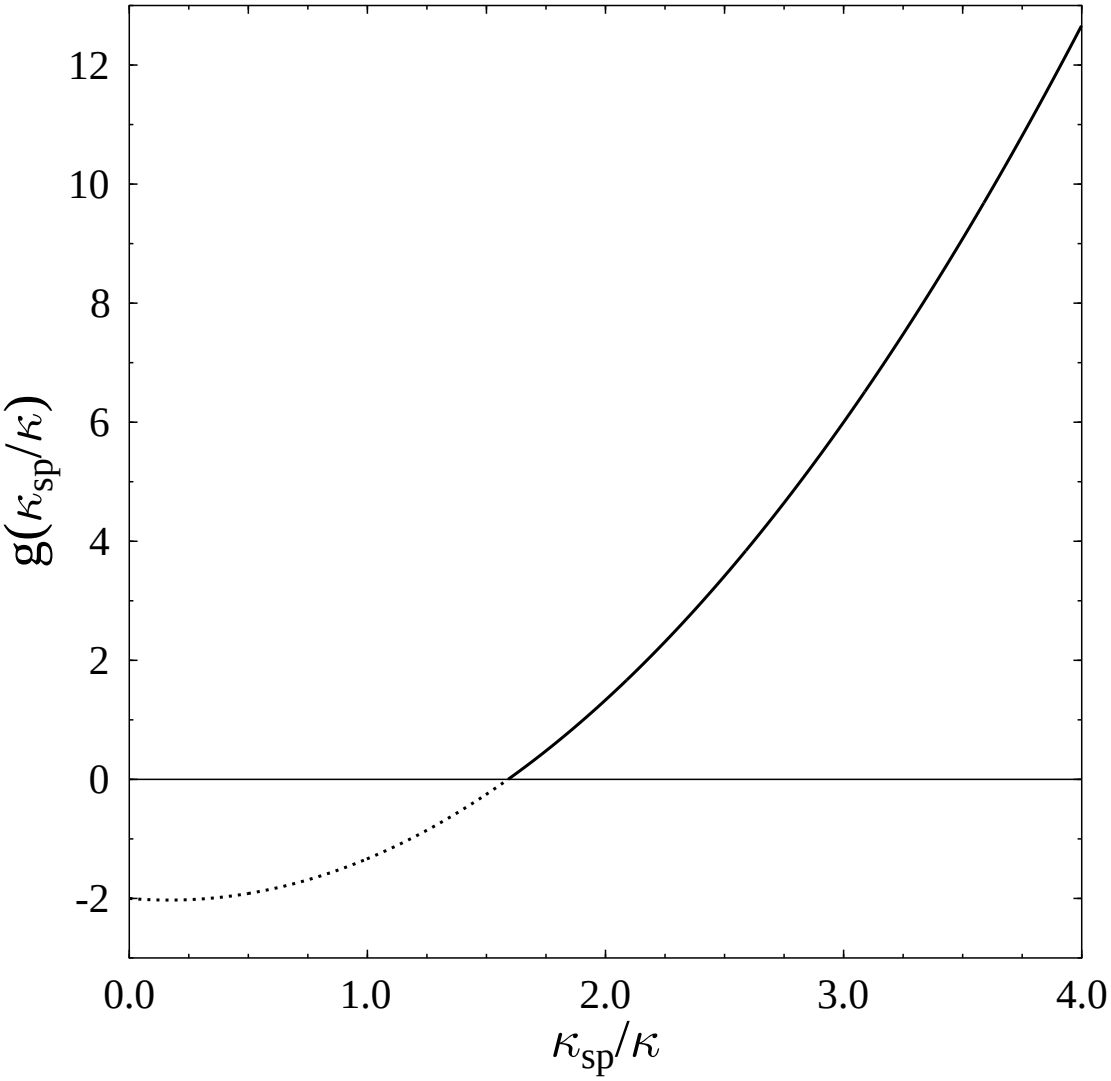
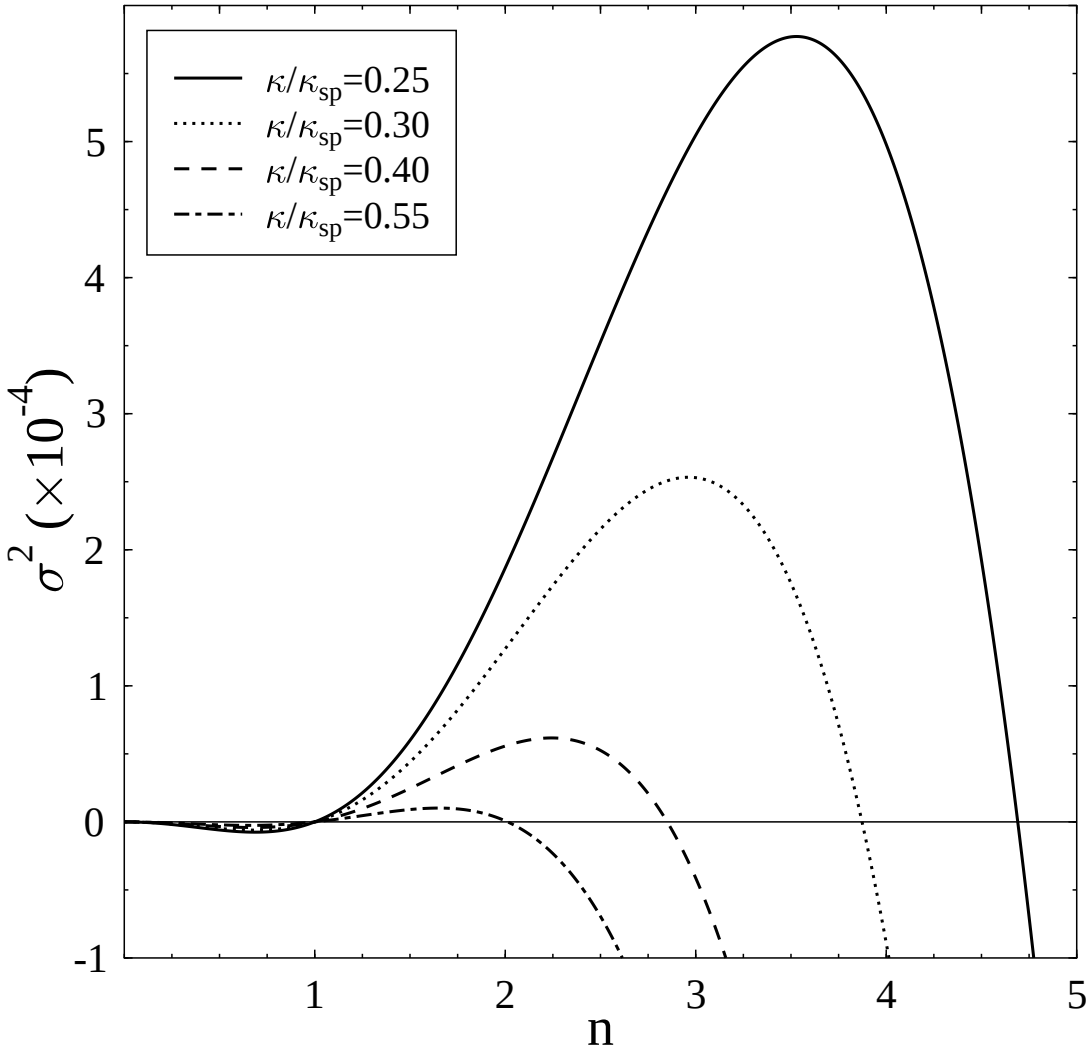
FIGURES

FIG. 1. The behavior of g [Eq. (22)] for $n = 2$ and $\Gamma = 2/3$. g is negative for $\kappa_0/\kappa \leq 1$ (the dotted part of the line), it becomes positive only when κ_0/κ exceeds some threshold value higher than 1 (the solid part). $g(\kappa_0/\kappa = 1) = -\Gamma(n^2 - 1)$ and is negative for the important case of $n \geq 2$. Thus it is obvious that buckling process can take place only for $\kappa < \kappa_0$. This prediction is confirmed by experiment.[1,2]

FIG. 2. The relation between the largest solution of $\Delta_{L_1}(\sigma) = 0$ [Eq. (20)] and n, at $\kappa/\kappa_0 = 0.25$ (the solid line), 0.30 (the dotted line), 0.40 (the dashed line), and 0.55 (the dot-dashed line) for the 168-bp DNA ring. We set $\kappa = \pi/(0.34 * 168)$ for the 168-bp DNA[10,12–15] and choose $\Gamma = 2/3$.[10,15] The most dominant deformation mode determined by the peaks of these curves increases with the decreasing of κ/κ_0, and the number of observable modes also increases as κ/κ_0 decreases. At $\kappa/\kappa_0 = 0.25$, the dominant mode is $n = 4$ and the modes $n = 2, 3, 4$ can be observed; while at $\kappa/\kappa_0 = 0.55$, no deformation mode with $n \geq 2$ will be excited. This prediction is in very close agreement with experimental observations.[2]


12
10
8
6
4
2
0
-2
0.0
1.0
2.0
3.0
4.0
$g(\kappa_{sp}/\kappa)$
κ_{sp}/κ


κ/κ_{sp}=0.25
κ/κ_{sp}=0.30
κ/κ_{sp}=0.40
κ/κ_{sp}=0.55
σ^2 ($\times 10^{-4}$)
n
-1
0
1
2
3
4
5
1
2
3
4
5